

# Peculiar Nature of Snake States in Graphene

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We study the dynamics of the electrons in a non-uniform magnetic field applied perpendicular to a graphene sheet in the low energy limit when the excitation states can be described by a Dirac type Hamiltonian. We show that as compared to the two-dimensional electron gas (2DEG) snake states in graphene exhibit peculiar properties related to the underlying dynamics of the Dirac fermions. The current carried by snake states is locally uncompensated even if the Fermi energy lies between the first non-zero energy Landau levels of the conduction and valence bands. The nature of these states is studied by calculating the current density distribution. It is shown that besides the snake states in finite samples surface states also exist.

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In recent experiments on graphene new transport phenomena resulting from the massless Dirac fermion type excitations have been observed generating huge interest both experimentally and theoretically [1, 2, 3]. For reviews on graphene see Refs. 4, 5, 6 and a special issue in Ref. [7].

While for 2DEG a number of experimental and theoretical works have been devoted to study the excitation spectrum of electrons and their transport properties in non-uniform magnetic fields, only a little is known about graphene in this case. For example, in 2DEG a special state called snake state exists in non-uniform magnetic field at the boundary where the direction of the magnetic field changes. The snake states in 2DEG were first studied theoretically by Müller [8] and it inspired numerous theoretical and experimental works (see, eg, Ref. [9] and references therein). The effect of an inhomogeneous magnetic field on electrons has been much less investigated in graphene. Martino et al. have demonstrated that the massless Dirac electron can be confined in inhomogeneous magnetic field [10]. Tahir and Sabeeh have studied the magneto-conductivity of graphene in a spatially modulated magnetic field and shown that the amplitudes of the Weiss oscillation are larger than that in 2DEG [11]. The low energy electronic bands have been studied by Guinea et al. [12] taking into account the non-homogeneous effective gauge field due to the ripples of the graphene sheet. However, snake states have been studied only in carbon nanotubes very recently by Nemec and Cuniberti [13].

In this work we study the electronic properties of graphene in a non-uniform magnetic field as shown in Fig. 1. We show the existence of snake states exhibiting peculiar behaviour at low energy. In particular, we find that these snake states are localized in the zero magnetic field region and carry current which is compensated at the edges of the sample far from the central region.

To study the nature of the snake states in graphene we consider a simple step like, non-uniform magnetic

field applied perpendicular to the graphene. The Dirac

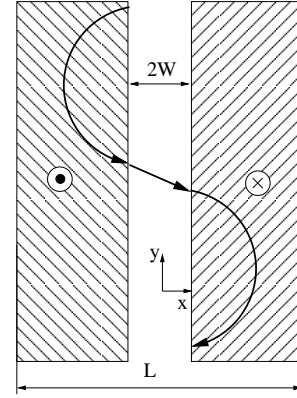


FIG. 1: The magnetic field applied perpendicular to the graphene is zero in the center region of width  $2W$ , and at the two sides of the strip they are in opposite directions with the same magnitude  $B$ . The total width of the strip is  $L \gg W$ . The classical trajectory of a typical snake state is also drawn schematically.

Hamiltonian of graphene in low energy approximation reads  $H_{\pm} = v(\sigma_x \pi_x \pm \sigma_y \pi_y)$ , where the index  $+$  ( $-$ ) corresponds to the valley  $\mathbf{K}$  ( $\mathbf{K}'$ ), the Fermi velocity is  $v = \sqrt{3}/2 a \gamma / \hbar$  given by the coupling constant  $\gamma$  between the nearest neighbours in graphene ( $a = 0.246$  nm is the lattice constant in the honeycomb lattice), while  $\boldsymbol{\pi} = (\pi_x, \pi_y) = \mathbf{p} - e\mathbf{A}$  is given by the canonical momentum  $\mathbf{p}$  and the vector potential  $\mathbf{A}$  related to the magnetic field as  $\mathbf{B} = \text{rot}\mathbf{A}$ . The Pauli matrices  $\sigma_x$  and  $\sigma_y$  act in the pseudo-spin space. The Hamiltonian is valley degenerate for arbitrary magnetic field, ie,  $\sigma_x H_{\pm} \sigma_x = H_{\mp}$ , therefore it is enough to consider only one valley. In what follows we take valley  $\mathbf{K}$ .

The energy spectrum of our system can be obtained from the Schrödinger equation  $H_+ \Psi(x, y) = E \Psi(x, y)$ . In our analytical calculations we assumed that  $L \gg l$ , where  $l = \sqrt{\hbar/|eB|}$  is the magnetic length. To construct

the wave function in each region we utilize the symmetries of the system. The system is translation invariant in the  $y$  direction and  $[H, p_y] = 0$  in Landau gauge if the vector potential has a form  $\mathbf{A} = (0, A_y(x), 0)^T$ . Therefore the wave function can be separated:  $\Psi(x, y) = \Phi(x)e^{iky}$ , where  $k$  is the wave number along the  $y$  direction. One can also show that  $[H, \sigma_y T_x] = 0$ , where  $T_x$  is the reflection operator, ie, it acts on an arbitrary function  $f(x)$  as  $T_x f(x) = f(-x)$ . This implies that the wave functions  $\Phi(x)$  can be classified as even wave functions satisfying  $\sigma_y T_x \Phi^{(e)}(x) = \Phi^{(e)}(x)$  and odd functions, when  $\sigma_y T_x \Phi^{(o)}(x) = -\Phi^{(o)}(x)$ . Moreover, it is true that  $[\sigma_y T_x, p_y] = 0$ . From these commutation relations the even (odd) wave function ansatz in the three different regions can be constructed. In the central region, ie, for  $|x| \leq W$  and at energy  $E$  it is given by

$$\Phi_C^{(e)}(x) = c_1 \left[ \begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix} e^{iKx} - i \begin{pmatrix} e^{i\varphi} \\ -1 \end{pmatrix} e^{-iKx} \right], \quad (1a)$$

$$\Phi_C^{(o)}(x) = c_1 \left[ \begin{pmatrix} 1 \\ e^{i\varphi} \end{pmatrix} e^{iKx} + i \begin{pmatrix} e^{i\varphi} \\ -1 \end{pmatrix} e^{-iKx} \right], \quad (1b)$$

where  $\tan \varphi = k/K$ ,  $K = \sqrt{\varepsilon^2 - k^2}$  is the transverse wave number and  $\varepsilon = E/(\hbar v)$ . In the left hand side, ie, for  $x \leq -W$  the wave function in Landau gauge reads

$$\Phi_L^{(e)}(x) = c_2 \begin{pmatrix} U(a_+, \xi) \\ \eta U(a_-, \xi) \end{pmatrix}, \quad \Phi_L^{(o)} = \Phi_L^{(e)}, \quad (1c)$$

where  $\xi = -\sqrt{2}(x + W + kl^2)/l$ ,  $a_{\pm} = (\pm 1 - \varepsilon^2 l^2)/2$ ,  $\eta = -i\sqrt{2}/(\varepsilon l)$ , and  $U(a, x)$  is a parabolic cylinder function[14] (from the two parabolic cylinder functions we take that which tends to zero for  $x \rightarrow -\infty$ ). The wave function ansatz in the right region, ie, for  $x \geq W$  can be obtained from  $\Phi_L^{(e,o)}(x)$  as  $\Phi_R^{(e)}(x) = \sigma_y T_x \Phi_L^{(e)}(x)$  and  $\Phi_R^{(o)}(x) = -\sigma_y T_x \Phi_L^{(o)}(x)$ . When  $k > \varepsilon$ , the above given transverse wave number  $K$  has to be replaced by  $K = -i\sqrt{k^2 - \varepsilon^2}$ . The boundary conditions require the continuity of the wave function at  $x = \pm W$  resulting in a homogeneous system of equations for the amplitudes  $c_1$  and  $c_2$ . Hence, nontrivial solutions can be obtained from the secular equation resulting in energy bands  $E_n(k)$  labelled by  $n = 0, \pm 1, \dots$  for a given  $k$ . Owing to the chiral symmetry ( $\sigma_z H_{\pm} \sigma_z = -H_{\pm}$ ) we have  $E_{-n}(k) = -E_n(k)$ [15].

Figure 2 shows the comparison of energy bands  $E_n(k)$  around the  $\mathbf{K}$  point obtained from the Dirac equation and from tight binding (TB) model. Note that our TB calculation is similar to that made by Wakabayashi et al. except that they applied uniform magnetic field [17]. In the figure the surface states calculated from TB model are not shown. This will be discussed below. The energies are scaled in units of  $\hbar\omega_c$ , where  $\hbar\omega_c = \sqrt{2}\hbar v/l = \sqrt{3/2}\gamma a/l$ . One can see that the agreement between the two calculations is excellent. For large enough positive

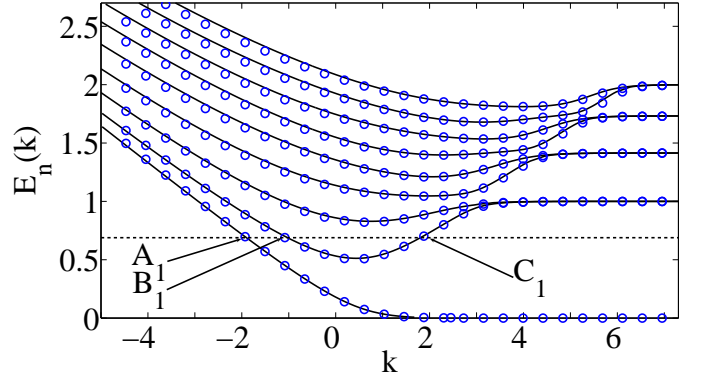


FIG. 2: The energy bands  $E_n(k)$  (in units of  $\hbar\omega_c$ ) as a function of  $k$  (in units of  $1/W$ ) around the  $\mathbf{K}$  point for magnetic field corresponding to  $W/l = 2.2$ . The solid lines (open circles) are the results obtained from the Dirac equation (TB model, [16]). Only the conduction band ( $E_n(k) \geq 0$ ) with  $n = 0, 1, \dots, 8$  states is shown ( $n = 0$  corresponds to the lowest conduction subband, and the other bands are in increasing order in energy). The even (odd) wave function states correspond to even (odd) quantum number  $n$ . States  $A_1$ ,  $B_1$  and  $C_1$  at energy  $0.688 \hbar\omega_c$  (dotted line) are snake states (see the text).

$k$  each state evolves into dispersionless, twofold degenerate Landau levels having the same energies as in uniform magnetic field, ie,  $E_n^L(k) = \text{sgn}(n) \hbar\omega_c \sqrt{|n|}$  with  $n = 0, \pm 1, \dots$ , where  $\text{sgn}(\cdot)$  is the sign function (see, eg, Ref. [15, 18]). However, for negative wave number  $k$  the energy bands are dispersive. Examples for such states are  $A_1$ ,  $B_1$  and  $C_1$  in Fig. 2. Each of these states carries current in the  $y$  or  $-y$  direction depending on their group velocity. The corresponding wave functions are localized in the central, zero magnetic field region as shown below (see Fig. 3). These are the snake states in our system.

It is also clear from Fig. 2 that the number of left and right moving states at a given energy are not the same which seems paradoxical at first sight. The ground state of the system appears to be unstable thermodynamically because there is a net current flow in the  $-y$  direction even in equilibrium. To understand this paradox one needs to consider the surface states localized at the edges of the system ( $x = \pm L/2$ ). Figure 3 shows the same energy bands  $E_n(k)$  as in Fig. 2 obtained from TB calculations for all allowed  $k$ . Two extra subbands appear and the resulting states at a given energy are denoted by  $D_1$  and  $D_2$  in Fig. 3 (although they are hardly distinguishable because of the parameters we used, see the caption of Fig. 2). We shall show that these non-degenerate states are surface states caused by the finiteness of the sample in the  $x$  direction and carry current in the  $y$  direction at the two edges, respectively. Moreover, in Fig. 3 states  $A_{1,2}$ ,  $B_{1,2}$ , and  $C_{1,2}$  are snake states and the first two states carry current in the  $-y$ , while  $C_{1,2}$  in the  $y$  direction. For finite  $L$  the surface states at the edges of the

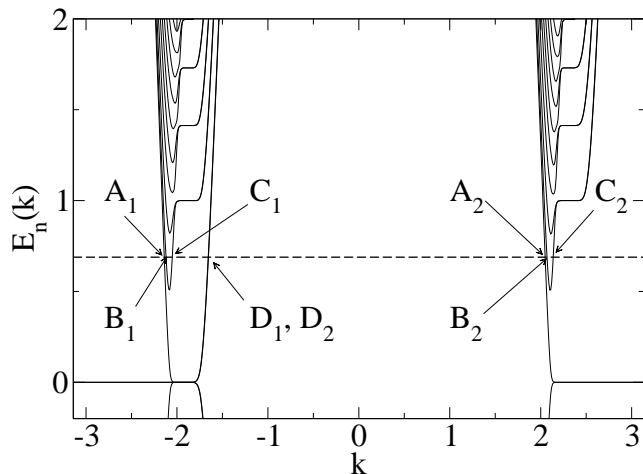


FIG. 3: The dispersion relation  $E_n(k)$  for all allowed  $k$  (in units of  $1/a$ ) including a small portion of the valence bands. The parameters are the same as in Fig. 2 for TB calculation. At the same energy as in Fig. 2 indicated by dashed line there are eight states:  $A_i$ ,  $B_i$ ,  $C_i$  and  $D_i$  with  $i = 1, 2$  (see the text).

sample will compensate the net current carried by the snake states. It is easy to see that including the surface states the number of left and right moving states are the same for all energies ensuring a stable equilibrium state of the system. We expect the same result using the Dirac Hamiltonian for finite  $L$  (see works by Brey and Fertig, and Abanin et al. in Ref. [7]).

To get better insight into the nature of the snake and surface states we calculated the current density distribution of these states shown in Fig. 4. As can be seen from

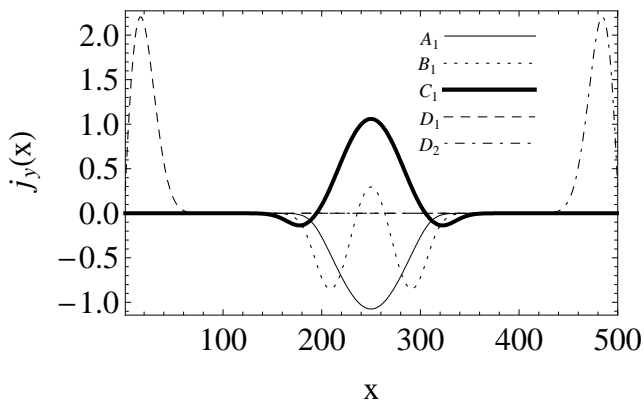


FIG. 4: Current density distributions  $j_y(x)$  (in arbitrary units) as a function of  $x$  (in units of lattice site in  $x$  ranging from 1 to  $N$ ) for states  $A_1$ ,  $B_1$ ,  $C_1$ ,  $D_1$  and  $D_2$  shown in Fig. 3.

the figure the snake states  $A_1$  and  $B_1$  carry current in the  $-y$  direction, while state  $C_1$  in the opposite direction. Moreover, all of these states are localized in the center of the sample. States  $D_1$  ( $D_2$ ) are surface states with current flowing in the  $y$  direction close to the left

(right) edges of the sample. States  $A_i$ ,  $B_i$  and  $C_i$  with  $i = 2$  behave the same way as that with  $i = 1$  due to valley degeneracy.

Varying the Fermi energy  $E_F$  the character of these states would change and consequently their current distribution too. For Fermi energy lying between the first and second Landau levels, ie, for  $E_0^L(k) < E_F < E_1^L(k)$  the net current contributing from snake states  $B_1$  and  $C_1$  localized at the center of the sample is zero, therefore they are locally compensated states. While the snake state  $A_1$  is also localized at the center, it is locally uncompensated. Only the current from surface state  $D_1$  will compensate the current from the snake state  $A_1$  to ensure the stability of the ground state of the system. However, locally this snake state is uncompensated since the overlap between states  $A_1$  and  $D_1$  is negligible. When the Fermi energy crosses the Landau level  $n = 1$  then not just state  $A_1$  but  $B_1$  also becomes uncompensated, while state  $C_1$  evolves into a surface state. Thus, we find that in graphene for all Fermi energies there is always at least one locally uncompensated snake state localized at the center of the sample and it is compensated only with surface states far from the center part of the system.

It is instructive to compare these results with that obtained for 2DEG with the same magnetic field profile as in Fig. 1. As can be seen from Fig. 5 the Landau levels

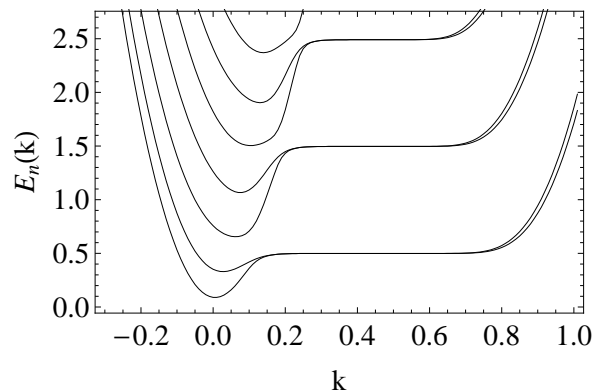


FIG. 5: The energy bands  $E_n(k)$  of 2DEG obtained from TB model for the same magnetic field profile as in Fig. 1 and with magnetic strength as in Fig. 2. The energies are in units of  $\hbar\Omega_c$ , where  $\Omega_c = eB/m$  with effective mass  $m$  of electrons, and  $k$  is in units of  $1/a$ , where  $a$  is the lattice constant in the square lattice). Here  $W = L/10$  and  $L = 200a$ .

are at energies  $E_n(k) = \hbar\Omega_c(n + 1/2)$ , where  $n = 0, 1, \dots$  as expected in case of uniform magnetic field. Using a similar analysis as before for graphene one can find snake and surface states [19]. The dispersion relation implies that in 2DEG no locally uncompensated current appears below the first Landau level ( $n = 0$ ). This is a striking difference between the two systems.

In summary, we studied the dynamics of electrons in graphene when the applied magnetic field is non-uniform.

For a simple, step-like magnetic field dependence we show that snake states appear similarly to the case of 2DEG. We calculated the energy bands in case of an infinite system using the Dirac Hamiltonian which agree very well with that obtained from our TB calculations. Moreover, we show that the surface states of a finite width sample ensure the stability of the ground state of the system. We find that in contrast to 2DEG the snake states in graphene are locally uncompensated for all Fermi energies. The different behavior of the snake states in graphene compared to the 2DEG is a clear manifestation of the massless Dirac fermion like excitations in graphene. The current carrying snake state at low enough Fermi energy (between the Landau level  $n = 0$  and  $n = 1$  or  $n = -1$ ) is expected to be as resilient against scattering on impurities as the surface states in quantum Hall effect of graphene. The peculiar behavior of the snake states in graphene with non-uniform magnetic fields could be utilized in future experimental and theoretical works.

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